Quasi-Chemical Model of Aqueous Solution Thermodynamics of Triflic Acid

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We present results of application of the quasi-chemical theory of statistical thermodynamics to the aqueous solution properties of triflic acid (trifluoromethane sulfonic acid, CF_3SO_3H). These quasi-chemical models are based upon extensive molecular orbital calculations on inner sphere clusters of water molecules with triflic acid and the triflate anion ($CF_3SO_3^-$) molecules together with dielectric models of outer sphere effects. Particular attention is given to comparison of the quasi-chemical model results with partial molar volumes, partial molar entropies, and equilibrium dissociation ($CF_3SO_3H + H_2O \leftrightarrow CF_3SO_3^- + H_3O^+$) ratios as a function of water activity. These thermodynamic properties will be used to model the water content of proton exchange membranes of Nafion® type as a function of water activity.